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Electronic structure calculations of Nitrogen and Hydrogen in diamond twist grain boundaries

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Films of ultrananoctrystalline diamond grown in methane/argon plasmas have grain sizes of 3 to 10 nm and show an increase of several orders of magnitude in *n*-type conductivity upon nitrogen addition to the plasma [Bhattacharyya *et al.*, Appl. Phys. Lett. **79**, 1441 (2001)]. Our computational studies have shown that nitrogen impurities are more stable in the grain boundaries than in the bulk. Using a density-functional-based tight-binding method, we have investigated the atomic and electronic structure of $\Sigma 13$ and $\Sigma 65-(100)$ diamond twist grain boundaries containing hydrogen and nitrogen at the same time. We have studied the formation of N–H complexes and associated changes in the electronic structure of the films for different hydrogen to nitrogen concentration ratios. We have also calculated participation ratios in order to find mobility edges in these systems and investigate the formation of defect sub-bands in the forbidden gap of diamond. These studies are being used to understand the experimentally observed changes in the electronic properties of the films associated with changes in the plasma composition during the growth process.

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Keywords

diamond, grain boundaries, electronic structure.